LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036243.D
Acq On : 20 Jun 2023 15:17
Operator : JC/MD
Sample : 03339-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-06

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Title : SW846 8260

Signal : TIC: VX036243.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.746	104	108	115	rVB	27932	38228	2.82%	0.295%
2	2.782	269	278	282	rBV	24740	54572	4.02%	0.421%
3	2.867	289	292	304	rVB3	12602	27317	2.01%	0.211%
4	3.105	321	331	345	rVB2	25936	63054	4.65%	0.486%
5	3.727	426	433	444	rVB4	7770	19289	1.42%	0.149%
6	4.209	501	512	520	rBV2	22553	64874	4.78%	0.500%
7	4.306	520	528	539	rVB4	27034	77760	5.73%	0.600%
8	5.123	650	662	671	rBV5	5738	23625	1.74%	0.182%
9	5.385	692	705	715	rBV2	86593	261954	19.30%	2.020%
10	5.550	723	732	739	rBV2	142152	405180	29.85%	3.124%
11	5.617	739	743	759	rVB3	71661	210375	15.50%	1.622%
12	5.830	767	778	788	rBV5	7996	24799	1.83%	0.191%
13	5.958	788	799	806	rVV	110309	300501	22.14%	2.317%
14	6.038	806	812	825	rVV2	44412	128229	9.45%	0.989%
15	6.251	825	847	858	rVV	129844	445054	32.79%	3.432%
16	6.355	858	864	874	rVB6	12283	35187	2.59%	0.271%
17	6.763	920	931	940	rBV	251589	621074	45.75%	4.789%
18	7.171	990	998	1007	rVB3	15543	32822	2.42%	0.253%
19	7.367	1019	1030	1041	rBV6	24770	74091	5.46%	0.571%
20	7.495	1044	1051	1057	rVV3	13082	28409	2.09%	0.219%
21	7.562	1057	1062	1065	rVV3	12794	27698	2.04%	0.214%
22	7.604	1065	1069	1074	rVV2	12723	27090	2.00%	0.209%
23	7.775	1090	1097	1104	rVB4	7011	15502	1.14%	0.120%
24	7.885	1111	1115	1122	rVB6	7150	14647	1.08%	0.113%
25	7.982	1122	1131	1141	rVB	117230	238272	17.55%	1.837%
26	8.104	1141	1151	1161	rBV	168649	361597	26.64%	2.788%
27	8.183	1161	1164	1179	rVB4	10385	28148	2.07%	0.217%
28	8.311	1179	1185	1192	rBV6	7493	17646	1.30%	0.136%
29	8.507	1208	1217	1227	rVB4	19202	39866	2.94%	0.307%
30	8.647	1227	1240	1247	rBV	505885	845729	62.30%	6.521%
31	8.720	1247	1252	1258	rVB	45975	69775	5.14%	0.538%
32	8.970	1288	1293	1299	rVB5	8197	17824	1.31%	0.137%
33	9.104	1307	1315	1320	rVB4	10236	20216	1.49%	0.156%
34	9.159	1320	1324	1328	rBV	26791	39246	2.89%	0.303%
35	10.055	1465	1471	1476	rBV	537601	716675	52.80%	5.526%
36	10.195	1490	1494	1499	rVB2	14226	21251	1.57%	0.164%

LSC Area Percent Report

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Operator : JC/MD
Sample : 03339-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Title : SW846 8260

37	10.299	1502	1511	1518	rVB	35351	57243	4.22%	0.441%
38	10.640	1561	1567	1573	rVB	10394	15478	1.14%	0.119%
39	10.963	1614	1620	1634	rBV	369874	482068	35.51%	3.717%
40	11.079	1634	1639	1644	rVV	422354	526290	38.77%	4.058%
41	11.122	1644	1646	1651	rVB	15686	17735	1.31%	0.137%
42	11.305	1666	1676	1684	rBV	689701	876184	64.55%	6.756%
43	11.482	1702	1705	1712	rVB4	8067	14263	1.05%	0.110%
44	11.610	1722	1726	1735	rVB	24222	33785	2.49%	0.261%
45	11.713	1735	1743	1746	rBV	9510	13673	1.01%	0.105%
46	11.750	1746	1749	1755	rVB2	10897	13607	1.00%	0.105%
47	11.866	1761	1768	1770	rBV	73254	97962	7.22%	0.755%
48	11.890	1770	1772	1776	rVB	62760	65085	4.79%	0.502%
49	12.018	1788	1793	1802	rBV	534227	685219	50.48%	5.284%
50	12.177	1816	1819	1824	rVB2	15931	19156	1.41%	0.148%
51	12.244	1824	1830	1837	rVV	1090563	1357459	100.00%	10.467%
52	12.311	1837	1841	1851	rVV2	123263	174908	12.88%	1.349%
53	12.402	1851	1856	1861	rVV	78819	99643	7.34%	0.768%
54	12.469	1862	1867	1873	rVB3	31222	46454	3.42%	0.358%
55	12.610	1885	1890	1894	rBV	405275	483430	35.61%	3.728%
56	12.646	1894	1896	1900	rVV	41452	41943	3.09%	0.323%
57	12.701	1900	1905	1912	rVB2	305236	444718	32.76%	3.429%
58	12.835	1919	1927	1932	rVB2	13525	21355	1.57%	0.165%
59	12.920	1932	1941	1947	rBV	277838	355979	26.22%	2.745%
60	13.024	1954	1958	1965	rVB3	27368	41536	3.06%	0.320%
61	13.116	1965	1973	1974	rBV3	20870	29169	2.15%	0.225%
62	13.164	1978	1981	1989	rVB	70076	102628	7.56%	0.791%
63	13.292	1998	2002	2007	rVB2	102875	141816	10.45%	1.094%
64	13.372	2012	2015	2020	rVB	14347	20388	1.50%	0.157%
65	13.420	2020	2023	2029	rVB	24923	32222	2.37%	0.248%
66	13.512	2029	2038	2040	rBV6	7762	15361	1.13%	0.118%
67	13.542	2040	2043	2046	rVV	28246	38579	2.84%	0.297%
68	13.579	2046	2049	2053	rVV2	38207	47239	3.48%	0.364%
69	13.640	2053	2059	2061	rVV2	21099	36126	2.66%	0.279%
70	13.670	2061	2064	2071	rVB2	26584	42436	3.13%	0.327%
71	13.774	2071	2081	2090	rBV	526621	660471	48.65%	5.093%
72	13.926	2098	2106	2110	rBV5	13032	22974	1.69%	0.177%
73	14.073	2125	2130	2136	rBV	22036	27654	2.04%	0.213%
74	14.213	2149	2153	2158	rBV3	18059	30748	2.27%	0.237%
75	14.317	2166	2170	2175	rBV	38705	50597	3.73%	0.390%
76	14.371	2175	2179	2185	rVB3	16463	23086	1.70%	0.178%

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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Title : SW846 8260

77	14.597	2209	2216	2219	rBV	14460	20973	1.55%	0.162%
78	14.634	2219	2222	2231	rVB2	18887	27258	2.01%	0.210%
79	14.780	2240	2246	2256	rVB	93555	125881	9.27%	0.971%
80	16.322	2492	2499	2510	rVB2	27203	50550	3.72%	0.390%

Sum of corrected areas: 12968905

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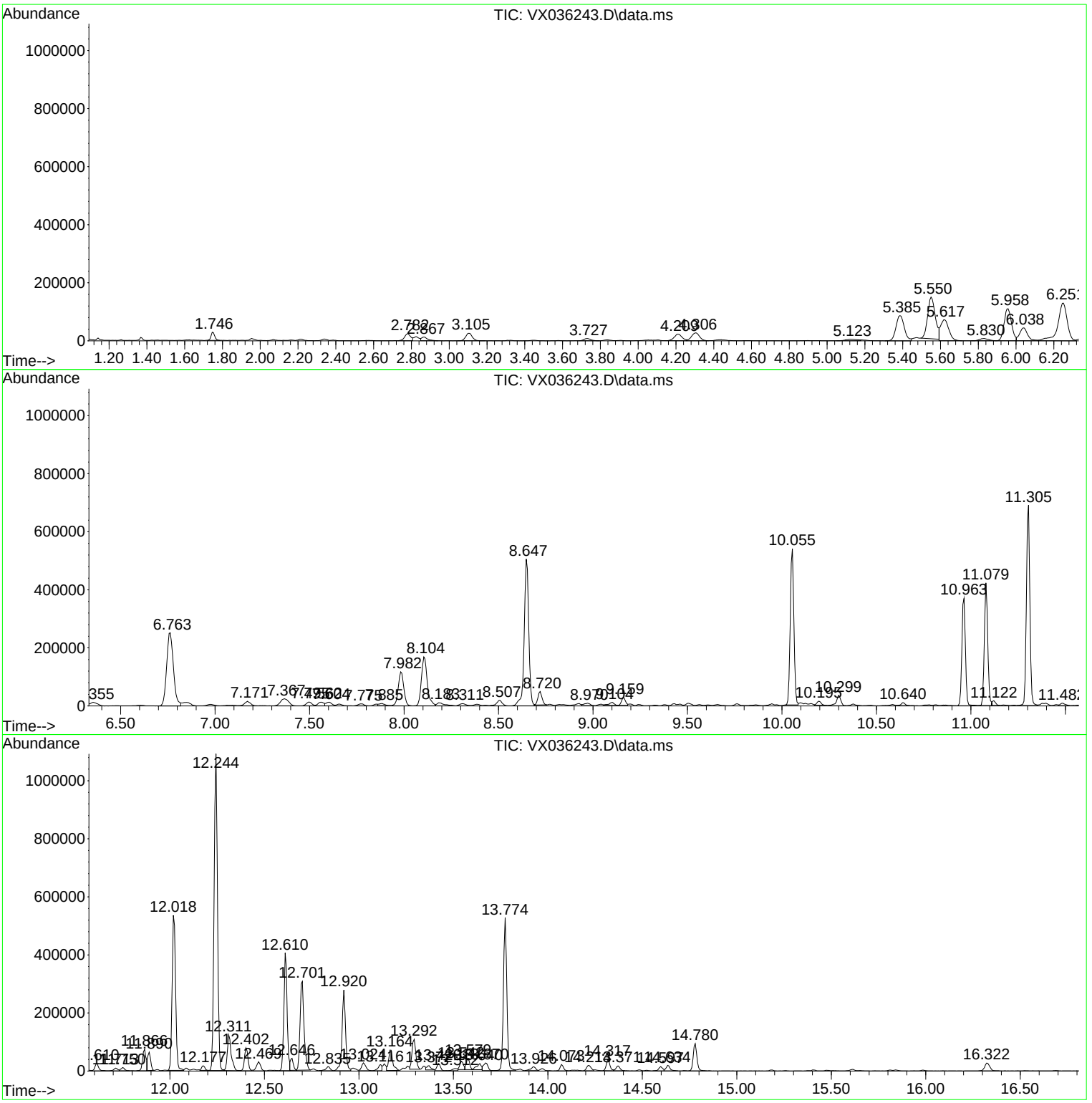
Instrument :
MSVOA_X
ClientSampleId :
MW-06

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036243.D
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Operator : JC/MD
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

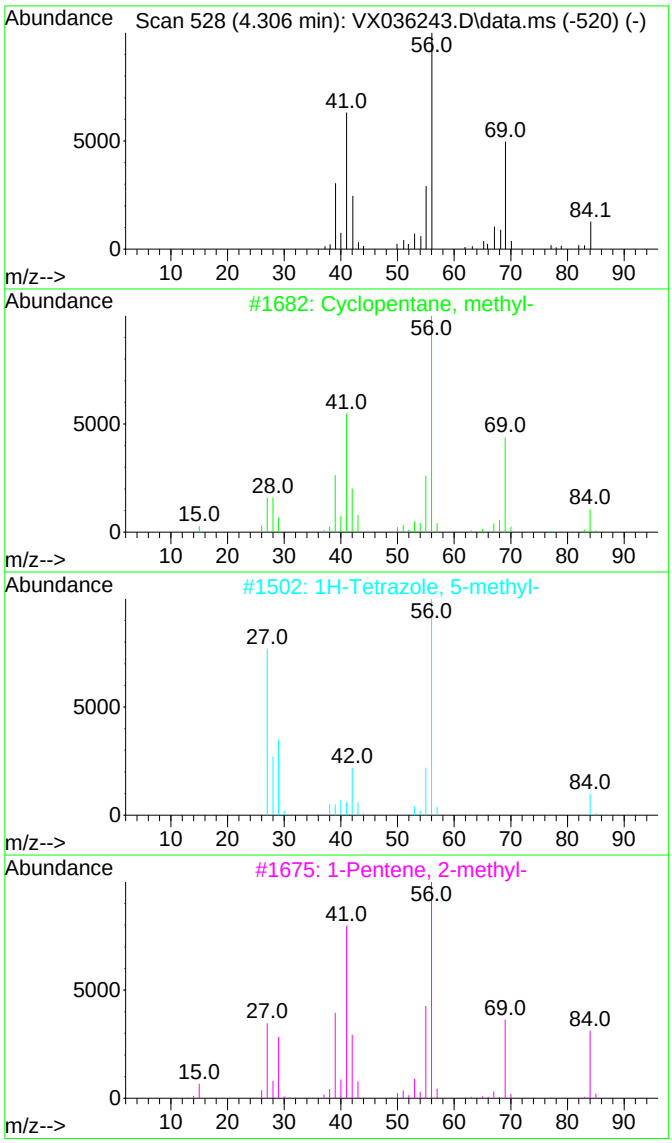
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

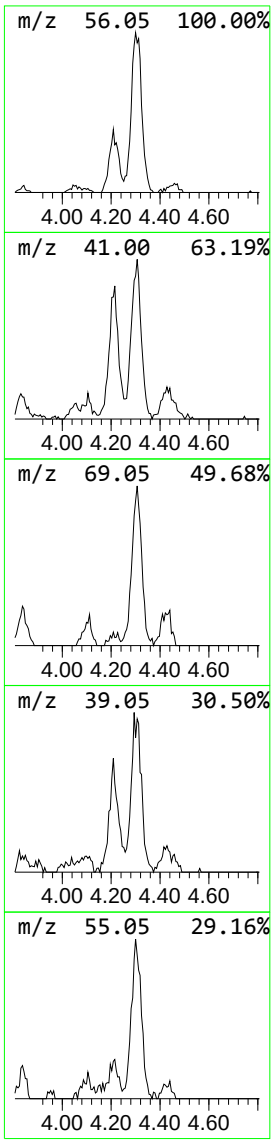
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	9.60 ug/l	77760	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	53
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	50
5	Cyclobutane	56	C4H8	000287-23-0	43





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

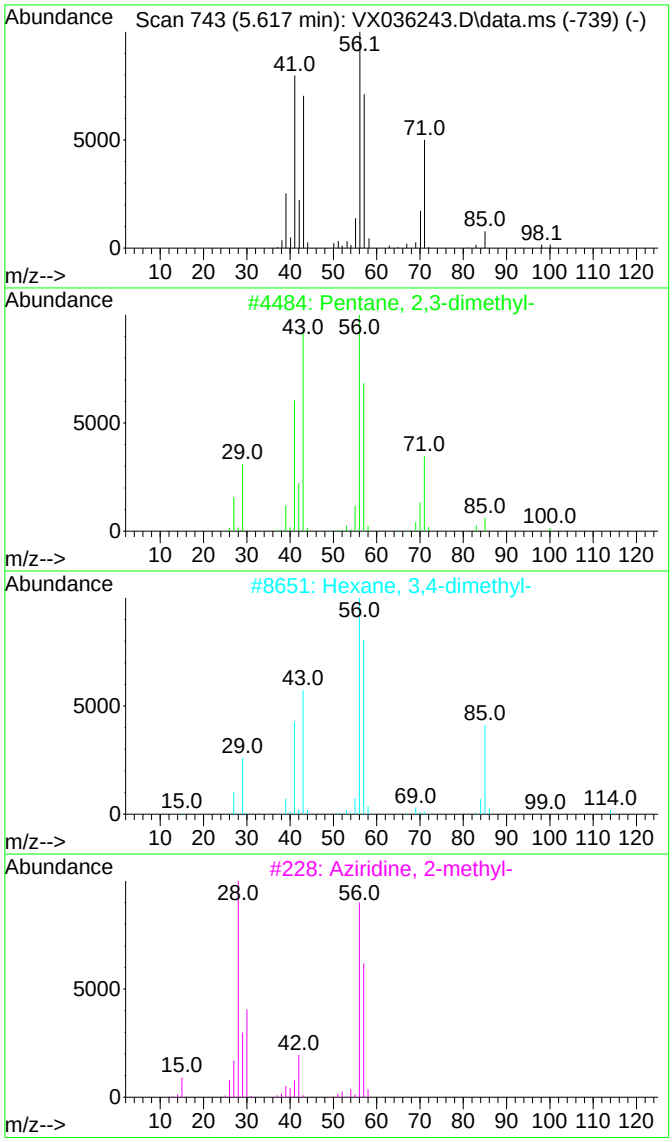
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

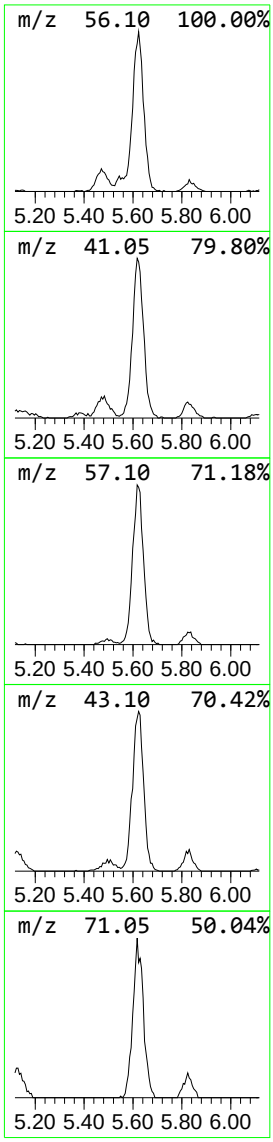
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.617	25.96 ug/l	210375	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	47
3	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
4	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	43
5	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036243.D
Acq On : 20 Jun 2023 15:17
Operator : JC/MD
Sample : 03339-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

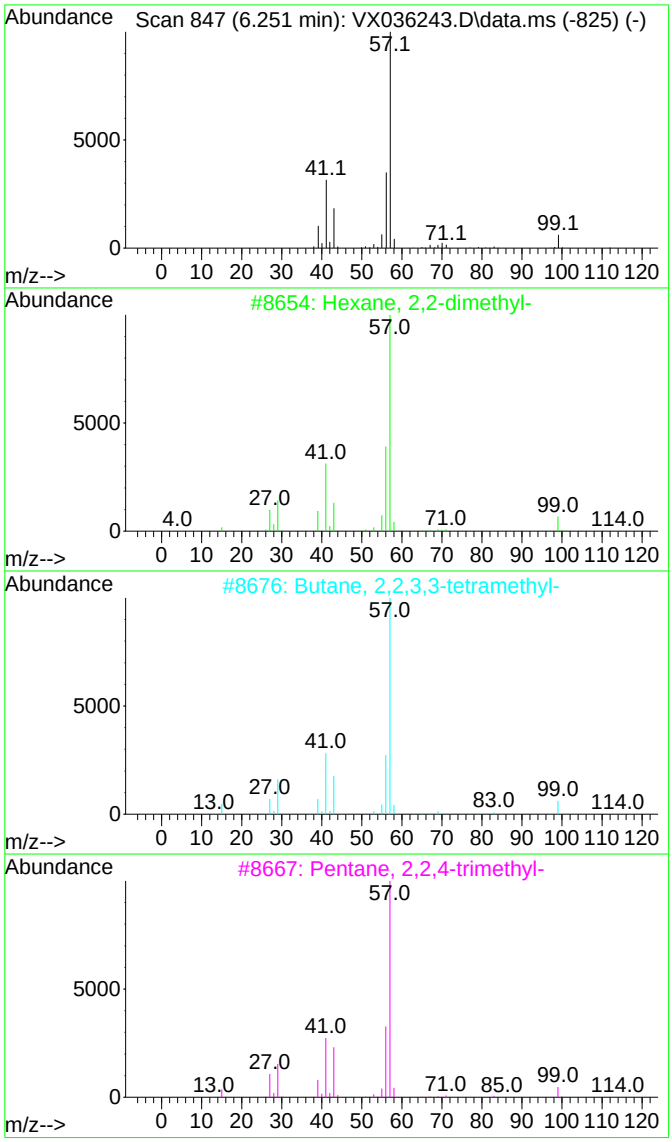
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

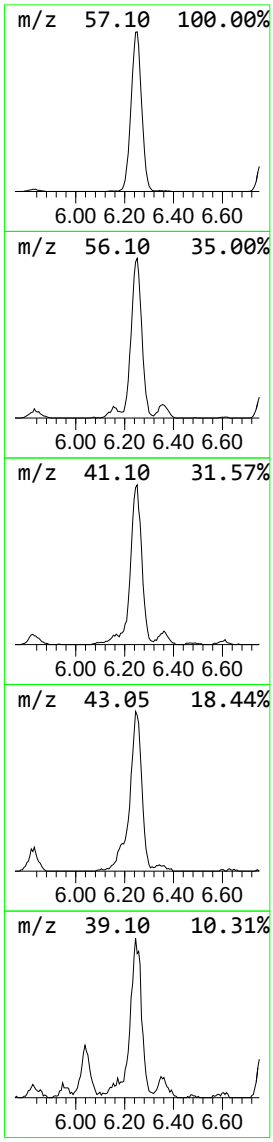
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexane, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	35.83 ug/l	445054	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
5	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	59





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MSVOA_X
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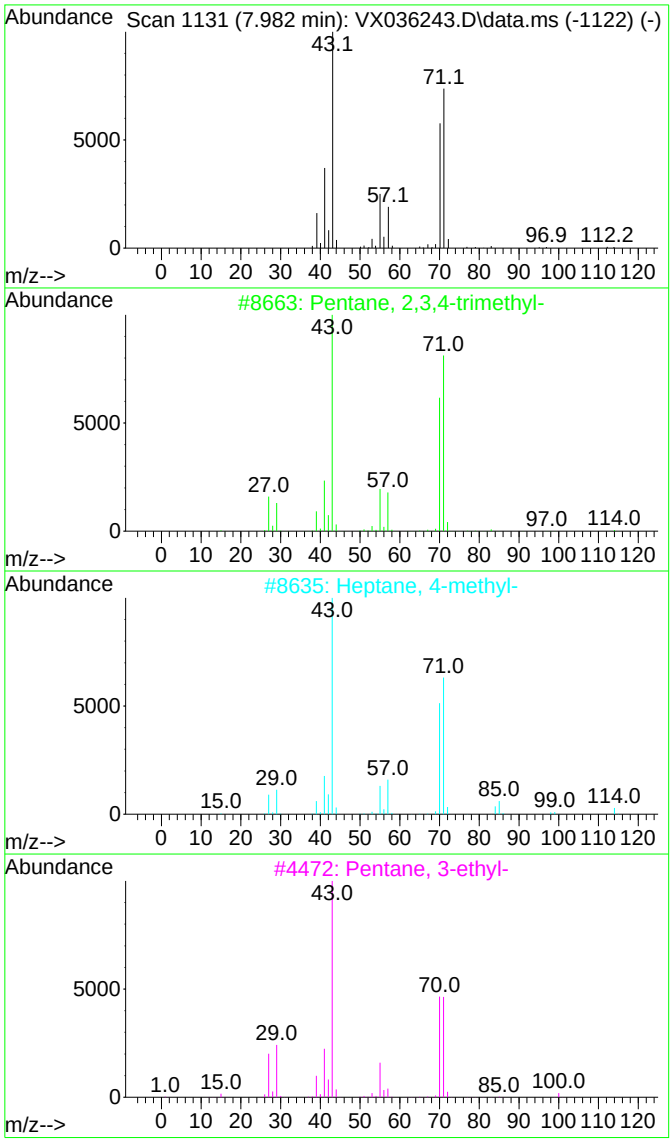
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

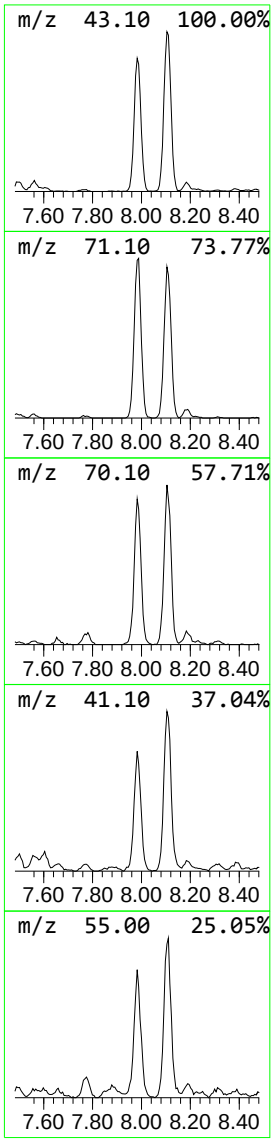
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.982	19.18 ug/l	238272	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	78





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

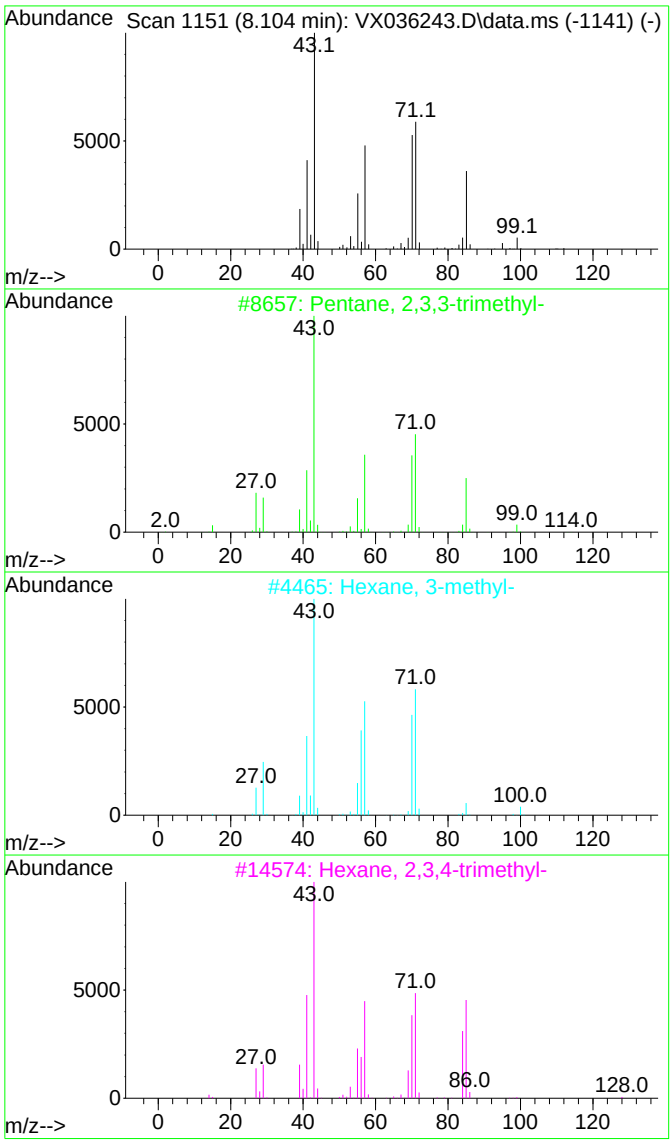
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

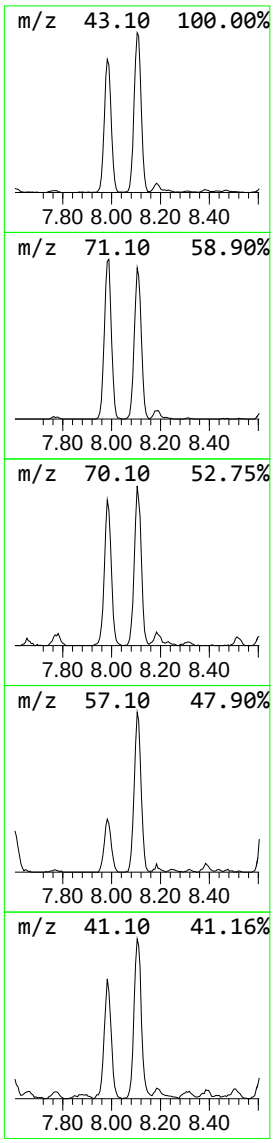
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 2,3,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	29.11 ug/l	361597	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	64
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

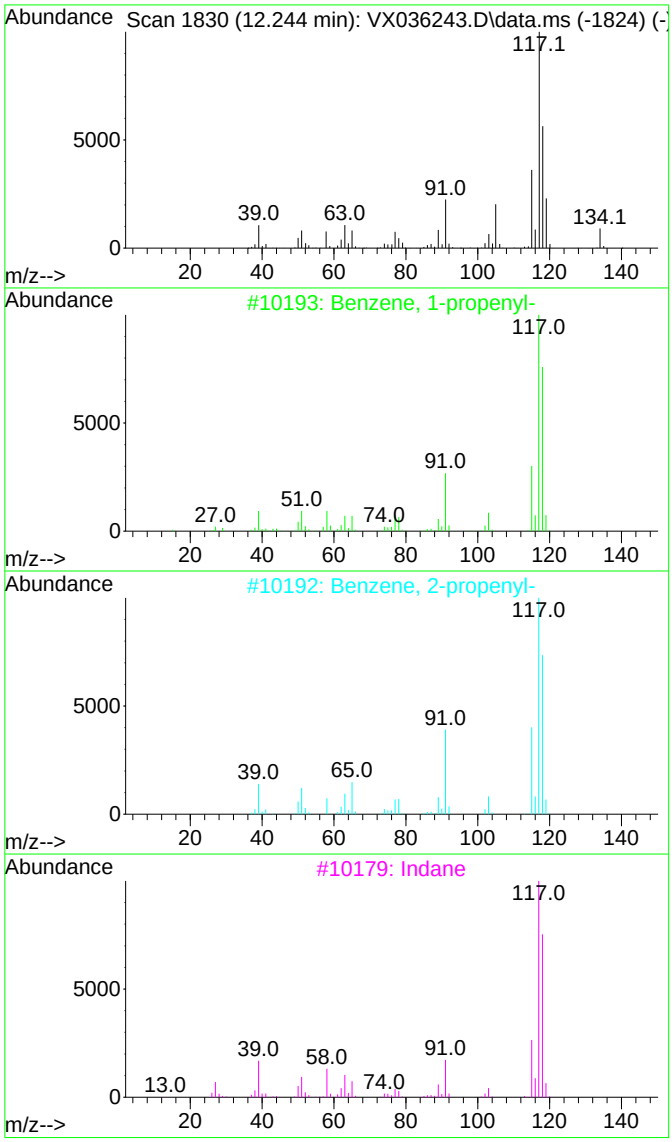
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

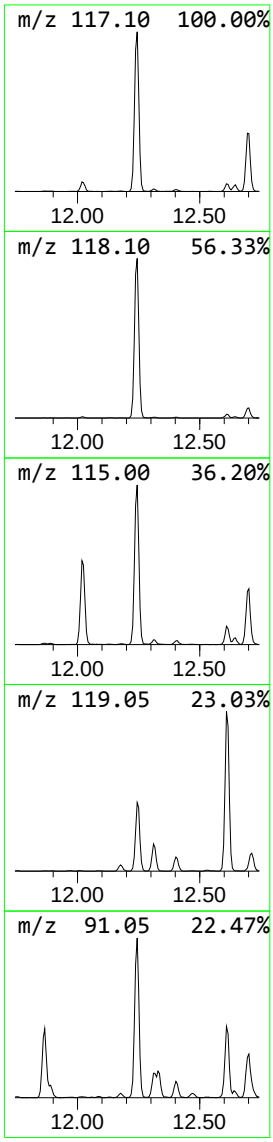
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-propenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	99.05 ug/l	1357460	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propenyl-	118	C9H10	000637-50-3	91
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
3	Indane	118	C9H10	000496-11-7	70
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036243.D
Acq On : 20 Jun 2023 15:17
Operator : JC/MD
Sample : 03339-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

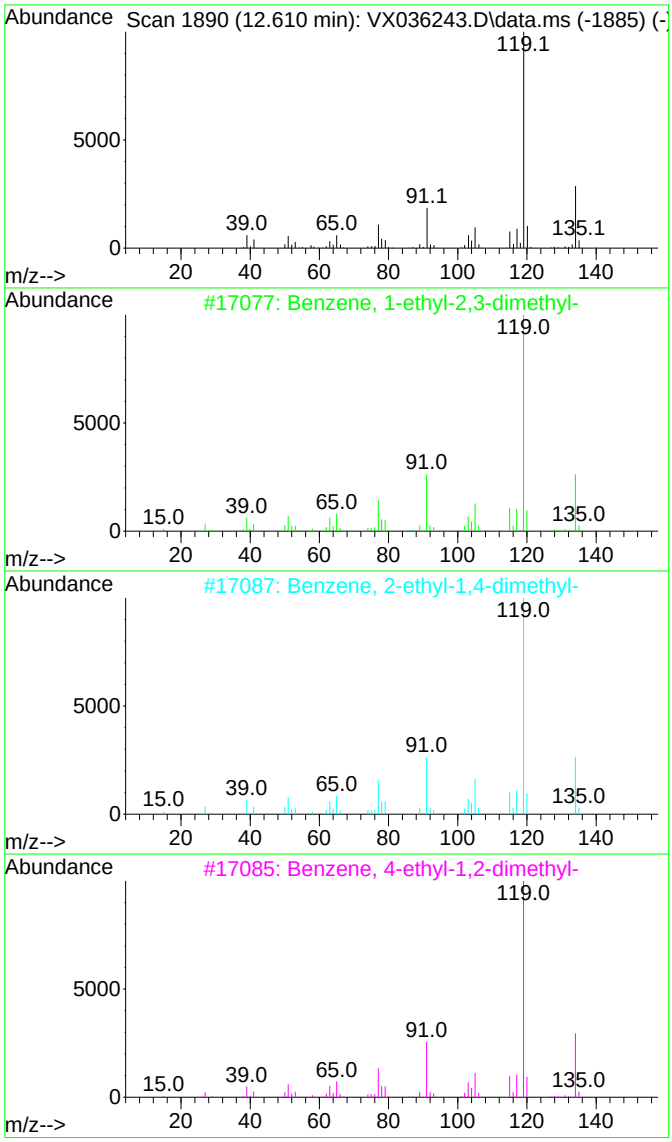
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

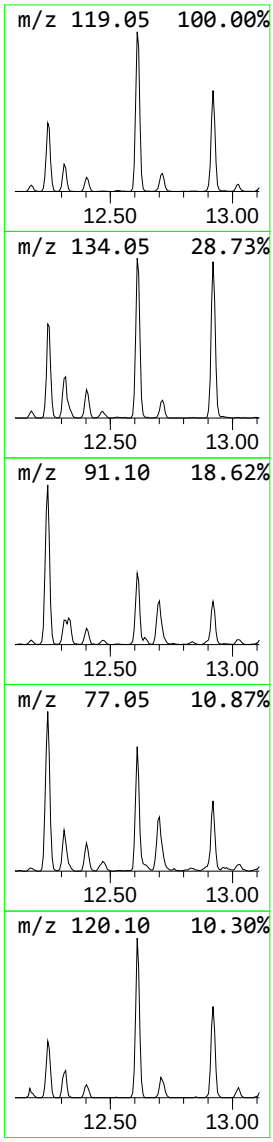
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	35.28 ug/l	483430	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
4	p-Cymene	134	C10H14	000099-87-6	95
5	o-Cymene	134	C10H14	000527-84-4	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036243.D
Acq On : 20 Jun 2023 15:17
Operator : JC/MD
Sample : 03339-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

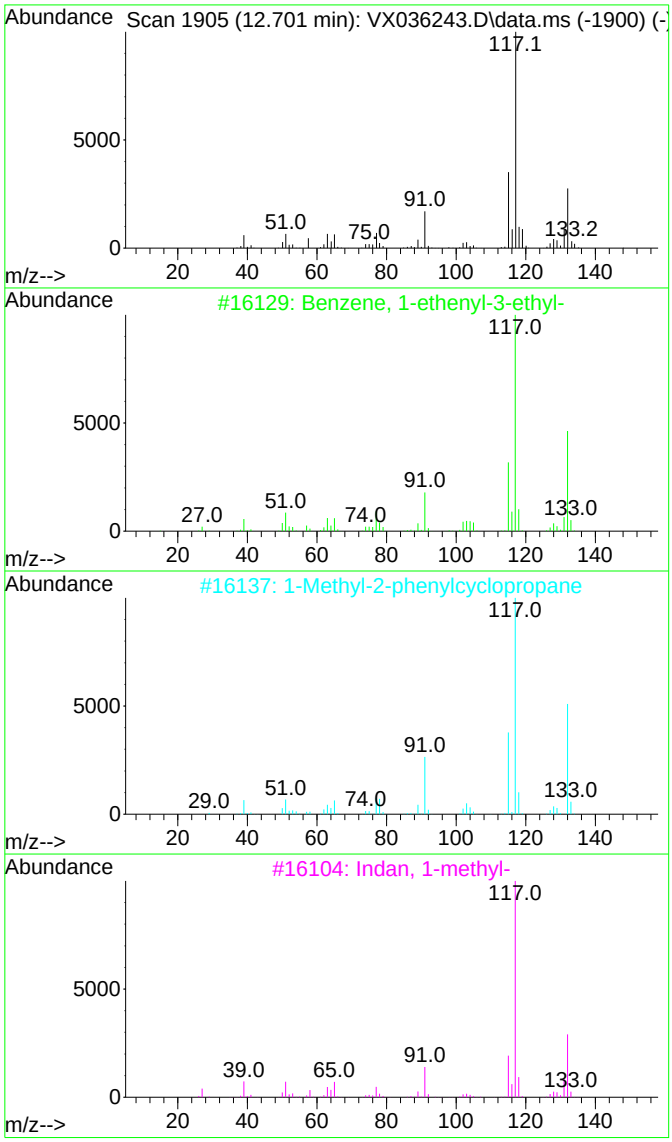
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

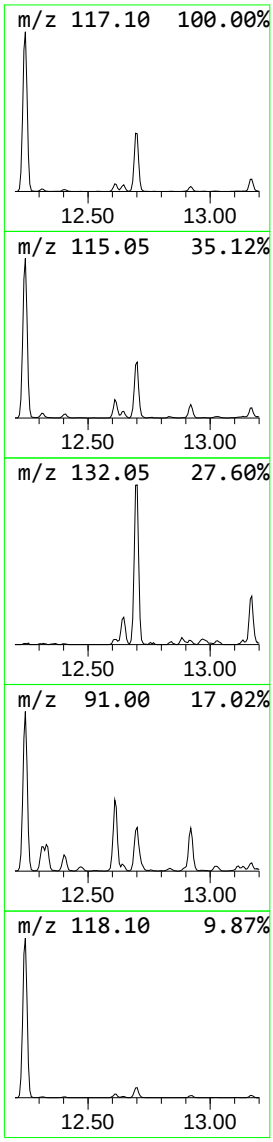
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	32.45 ug/l	444718	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036243.D
Acq On : 20 Jun 2023 15:17
Operator : JC/MD
Sample : 03339-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

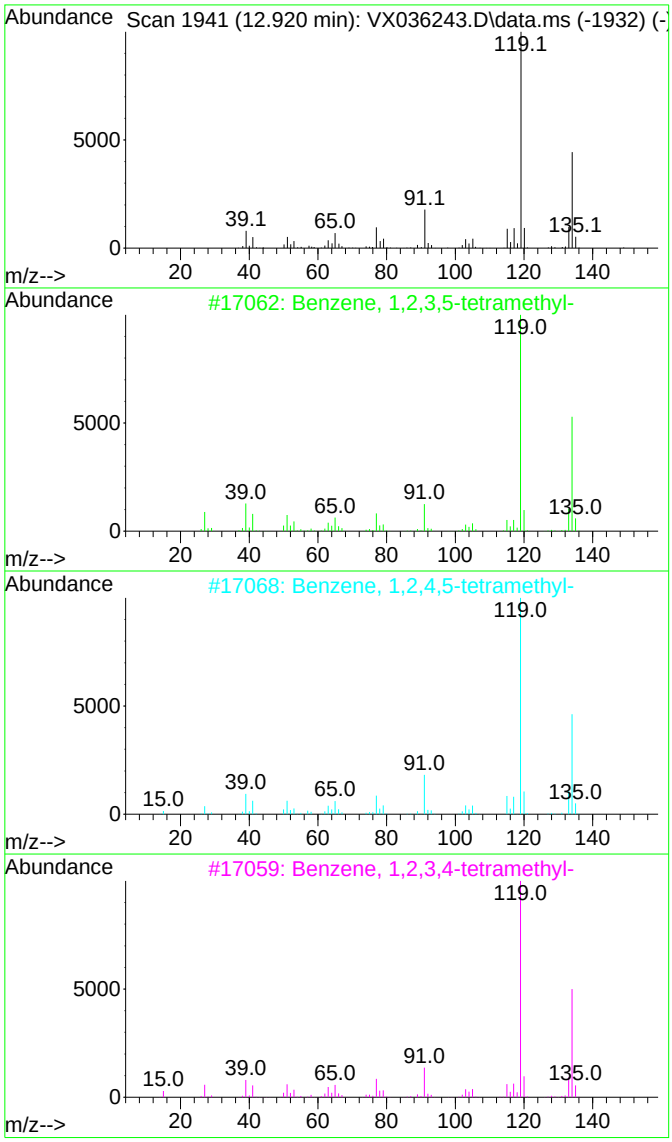
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

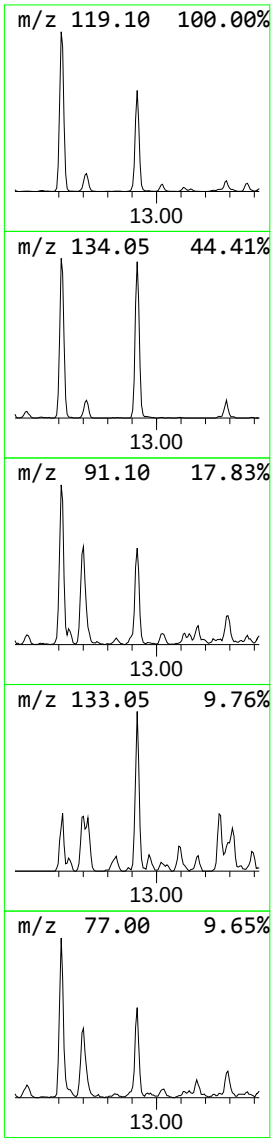
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	25.98 ug/l	355979	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036243.D
Acq On : 20 Jun 2023 15:17
Operator : JC/MD
Sample : 03339-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

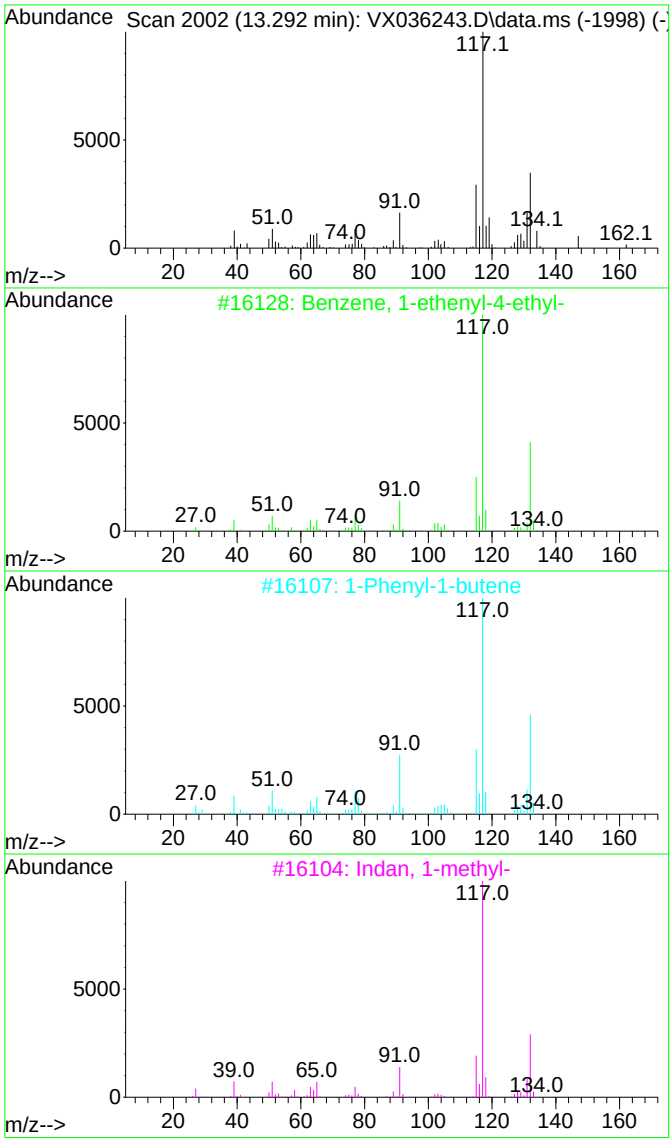
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

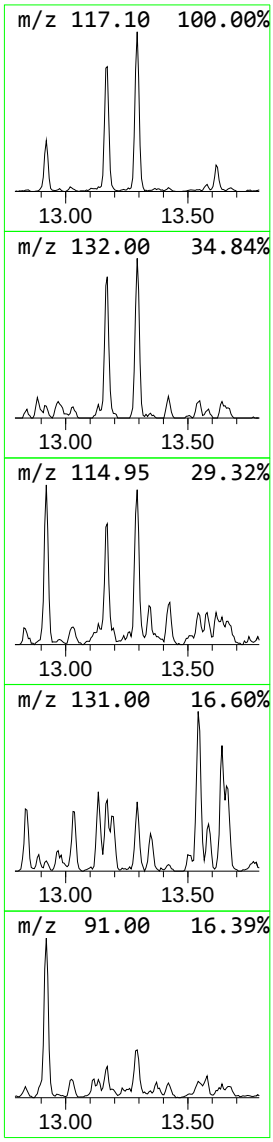
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	10.35 ug/l	141816	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	83
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062023\
Data File : VX036243.D
Acq On : 20 Jun 2023 15:17
Operator : JC/MD
Sample : 03339-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, m...	4.306	9.6	ug/l	77760	1	5.550	405180	50.0
Pentane, 2,3-di...	5.617	26.0	ug/l	210375	1	5.550	405180	50.0
Hexane, 2,2-dim...	6.251	35.8	ug/l	445054	2	6.763	621074	50.0
Pentane, 2,3,4-...	7.982	19.2	ug/l	238272	2	6.763	621074	50.0
Pentane, 2,3,3-...	8.104	29.1	ug/l	361597	2	6.763	621074	50.0
Benzene, 1-prop...	12.244	99.0	ug/l	1357460	4	12.024	685219	50.0
Benzene, 1-ethy...	12.610	35.3	ug/l	483430	4	12.024	685219	50.0
Benzene, 1-ethe...	12.701	32.5	ug/l	444718	4	12.024	685219	50.0
Benzene, 1,2,3,...	12.920	26.0	ug/l	355979	4	12.024	685219	50.0
Benzene, 1-ethe...	13.292	10.4	ug/l	141816	4	12.024	685219	50.0